**Close out and Final report for**
**NASA Glenn Cooperative Agreement NCC3-534**

**CFD Code Development for Combustor Flows**

## Introduction

This report summarizes the work performed by Dr. Andrew Norris under the NCC3-534 grant, from January 16, 1997 thru December 16, 2003. It includes a summary of each year's work, and also a list of publications.

## January 16, 1997–December 16, 1997

### *Manifold Reaction Schemes*

During the year, the Intrinsic Low-Dimensional Manifold code was developed. This code takes a full reaction mechanism, and automatically simplifies it into a reduced mechanism. The technique has the advantage of requiring no knowledge of detailed combustion chemistry, and also shows significant improvement in accuracy over existing reduced mechanisms. For example, the popular one-step schemes of Westbrook and Dryer are similar in complexity to the ILDM method, but over-predict adiabatic flame temperature by 100–200K and only contain information about the major species. The ILDM scheme however contains information about all the major and minor species, and so predicts the adiabatic flame temperature accurately.

Validation tests showed the accuracy of the ILDM scheme, parameterized by two scalars, to be of the same order of accuracy as a reduced mechanism containing 12 species and 10 rate equations for PSR calculations. The ILDM mechanisms are currently being applied to the National Combustor Code (NCC) project.

### *NOx Post-Processor*

The NOx Post processor, based on the ILDM reduced reaction scheme, was also worked on. Its capabilities were upgraded to include JetA as a fuel and is currently being used by Pratt and Whitney for pollutant prediction in their design codes.

### *PDF Code*

A calculation was performed using the LPDF2D code with improved CMOTT turbulence models to predict the flow in a can combustor. This work tested the turbulence models, and also the new convection schemes developed by for the PDF code. Results showed that with the improvements, the PDF part of the code only took 40% of the total CPU time required. This work was reported at the 1996 Joint Propulsion Conference.

***Publications***

A.T. Norris, *Application of Low Dimensional Manifolds in NOx Prediction,* 33rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Seattle, Washington, AIAA-97-3243, 1997

A.T. Norris, *Automated Simplification of Full Chemical Mechanisms.* 33rd AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Seattle, Washington, AIAA-97-3115, 1997

A.T. Norris, *Automated Simplification of Full Chemical Mechanisms: Tabulation Implementation*, Propulsion Engineering Research Center 9th Annual Symposium on Propulsion. Cleveland, Ohio, 1997

**December 16, 1997–December 16, 1998**

***Manifold Reaction Schemes***

During the year, further development of the Intrinsic Low-Dimensional Manifold code was undertaken. This code takes a full reaction mechanism, and automatically simplifies it into a reduced mechanism. Work performed consisted of numerical enhancement of the ILDM code, to provide a more friendly user interface. The proposed inclusion of the ILDM code in the LSENS code was postponed until the LSENS code has finished a major upgrade.

In addition the ILDM code was installed in the National Combustion Code, in both the scalar PDF and the conventional assumed PDF combustion modules. A separate interface was written for the assumed PDF calculations, and included in the ILDM package. Preliminary results for the ILDM scheme show a 75% reduction in CPU time compared to the 12 species chemistry package.

Validation tests showed the accuracy of the ILDM scheme, parameterized by two scalars, to be of the same order of accuracy as a reduced mechanism containing 12 species and 10 rate equations for PSR calculations. This work was reported at the 1997 Joint Propulsion Conference.

***Neural Network Reaction Storage***

In cooperation with ABtech corporation, an investigation was performed into the feasibility of using neural network techniques to store the reaction tables. Using this method we hope to eliminate the big problem of table storage: Memory limitations. The memory problems are based on the need to obtain a good resolution for the stored function, which requires many table entries. For example a table may require on order of 100 entries to resolve a particular component. If the table is just a function of two parameters, this gives a 10,000 element table. But if a table is to be the function of five

parameters, this corresponds to a 10,000,000,000 element table, or for one stored component, 40Gb of memory.

By using Neural network approaches, we hope to replace the whole table structure by a system of polynomial functions. This will eliminate the restriction on the number of parameters to describe the reaction, as the size of the polynomials is negligible. The speed of evaluating the polynomials will be more than the table look-up, but should be still significantly less than the conventional mechanisms. Initial work has shown that a good agreement can be obtained between the neural network results and the table. Currently the error estimates have the maximum error at about 5% compared to the table predictions.

***NOx Post-Processor***

The NOx Post processor, based on the ILDM reduced reaction scheme, was also worked on. It's capabilities were upgraded to include Jet-A as a fuel and is currently being used by Pratt and Whitney for pollutant prediction in their design codes. This method was reported at the 1997 Joint Propulsion Conference.

***Thermodynamic Approach to Reduced Chemical Kinetics***

During the year, some advances in the thermodynamic approach to simplifying chemical kinetics was made.

One can consider the composition of a mixture to be a point in N-dimensional scalar space, with N being the number of species. Thus if you change the composition due to reaction, this appears as the motion of the point to another location on the scalar space. Now at each point in the scalar space, there is a chemical potential, also known as the Gibbs free energy. There is also one point in the scalar space where this is minimum; the equilibrium point. The application of chemical kinetic mechanisms results in the composition to move toward this point.

The thermodynamic approach is based on the premise that if we know the species in the reaction, we can determine the Gibbs free energy field for the entire scalar space. As all chemical reactions consist of a motion from a high chemical potential to the minimum, the reaction rate kinetics may be replaced by a simple caternary-type argument. That is, why not just slide "downhill" to the minimum and use the resulting path as the kinetic scheme?

The main advantage in doing this is that the need for a complex "full" mechanism can be avoided. These "full" mechanism consist of hundreds of rate expressions, each with at least three constants that have to be determined. The creation of these mechanisms is very labor intensive, and the availability is limited.

Work to date has been mainly in the area of setting up the necessary numerical tools to analyze the resulting multi-dimensional spaces, and preliminary work on finding the potential and potential gradient.

***Publications***

A.T. Norris, *Automated Simplification of Full Chemical Mechanisms: Implementation in National Combustion Code*, 34th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Cleveland, Ohio, AIAA-98-3987, 1998

K.H. Chen, A.T. Norris, A. Quealy and N.S. Liu, *Benchmark Test Cases for the National Combustion Code*, 34th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Cleveland, Ohio, AIAA-98-3855, 1998

T.J. Van Overbeck and A.T. Norris, *An Evaluation of Stochastic Predictions of Hydrogen-Air Combustion*, 34th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Cleveland, Ohio, AIAA-98-3946, 1998

**December 16, ~~1998~~–December 16, ~~1999~~**

***Manifold Reaction Schemes***

Several significant steps were taking in the development of the Intrinsic Low-Dimensional Manifold code. This code takes a full reaction mechanism, and automatically simplifies it into a reduced mechanism.

Work performed consisted of introducing an adaptive tabulation scheme into the code, which provides an automatic way of ensuring a more uniform accuracy to the resulting table. This is achieved by placing more grid points in regions of strongly-varying chemical reaction, and so achieving better resolution in these regions.

A second major improvement was the extension of the tables to include super-equilibrium compositions. It is observed that mixing can produce chemical compositions that lie "above" the fully-burnt state, and so the ILDM code was re-written to include these regions. This involved utilization of Simplex schemes to establish the limits of composition space, and alteration to the storage methods.

During this time, the ILDM scheme was used in the NCC code for several different cases. Timing results for the code show significant benefits to the performance of NCC compared to using 12 species finite rate methods.

Implementation of ILDM in the NCC code and a comparison of the results obtained by a 12 step mechanism were reported for the case of a piloted methane flame at the 1998 Joint Propulsion Conference.

*Neural Network Reaction Storage*

No work was performed on the Neural Network storage of ILDM mechanisms. This part of the project was delayed a year to allow Abtech to port their program to the Unix environment. This work is expected to continue in 1999.

*PDF in NCC*

Late in 1998, Allison Gas Turbines provided us with a Scalar PDF solver. Currently this solver does not work in a multi-processor environment, and this is to be attempted in 1999.

*Thermodynamic Approach to Reduced Chemical Kinetics*

Last year, some numerical tools for the investigation of reaction kinetics were developed. Some further work on these was performed during the year.

Areas investigated included use of minimization techniques to find reaction paths, decomposition of composition space into orthogonal basis vectors and comparison with existing kinetic rate expressions. However no significant breakthroughs have been made so far.

*Publications*

A.T. Norris, *Extended ILDM Method for NCC*, 35th AIAA/ASME/SAE/ASEE Joint Propulsion Conference, Los Angeles, California, AIAA-99-2390, 1999

**December 16, 1999–December 16, 2000**

*Jacobian Evaluation of Manifolds for ILDM*

For this task, the development of an adaptive tabulation scheme was accomplished. How this differs from the existing version is that the new method allows full point-refinement, rather than requiring the sequential partial refinement of all points. The code for this is currently being verified. In addition, an existing Jacobian ILDM code has been obtained, and its suitability evaluated.

*ILDM Interactive Tabulation*

For this task, the first requirement is point-refinement adaptive tabulation scheme, and this was developed in conjunction with the previous task. Details of how this code should be altered for parallel computer architectures are currently being considered.

*Neural Network Reaction Storage*

Preliminary work was resumed on this task, which is currently being carried out in conjunction with Albert Huntington of Virginia Tech. He has been working closely with AbTech in developing neural models from data supplied by NASA. In turn, these neural models will be returned to NASA to be tested.

*PDF models in NCC*

Development of the PDF model was accomplished, with the standardization of the combustion modules, and physical properties. In addition a new convection scheme was coded, along with new time averaging and random number generation.

*User Interface*

The chemistry user interface for NCC has been streamlined, with the new input automatically assigning properties from the NASA thermodynamic database. In addition, significant portions of the chemistry routines have been re-written to accommodate the new method. Also a dedicated one-step global chemistry option has been added as an additional chemistry model.

*Validation*

Validation has been confined to testing the chemistry and input routines, and so has focused on simple flame problems.

*Publications*

A.T. Norris, K.H. Chen and M.S. Raju, *Chemical Kinetics in the National Combustion Code*, AIAA 38th Aerospace Sciences Meeting and Exhibit, Reno, Nevada, AIAA-2000-0334, 2000

A. Quealy, R. Ryder, A.T. Norris and N.S. Liu, *National Combustion Code: Parallel Implementation and Performance*, AIAA 38th Aerospace Sciences Meeting and Exhibit, Reno, Nevada, AIAA-2000-0336, 2000

T.-H. Shih, A.T. Norris, A. Iannetti, C.J. Marek, T.D. Smith, N.-S. Liu and L.A. Povinelli, *A Study of Hydrogen/Air Combustor Using NCC*, AIAA 39th Aerospace Sciences Meeting and Exhibit, Reno, Nevada, AIAA-2001-0808, 2001

**December 16, 2000–December 16, 2001**

*Code Development*

During the 2000–2001 year, a large portion of work was carried out in an overhaul of the thermal and transport properties portion of the NCC. In addition, the solver for the

chemistry source term was replaced, as this portion of the code was failing to provide accurate results.

For the transport and thermal properties, a significant amount streamlining was performed, with the aim of making the code more readable and simplifying the process of adding more modules. In addition, the Magnussen model was modified to allow the use of properties that vary with temperature. These changes have been tested and successfully implemented in the NCC. In addition, the new high-pressure equation of state model, provided by Dr. Raju was modified to conform to the new code structure.

For the chemistry source terms, the same input file as the finite rate mechanism and Westbrook and Dryer model now provides the input for the Magnussen model. This involved re-writing the chemistry pre-processor and also the input routines.

A significant amount of research was put into the performance of the chemistry source term integrator, used for the finite rate chemistry module. The existing integrator, a one-step implicit scheme, proved to be inaccurate for anything but very short time-steps. Other schemes were investigated, including the LSODE integrator, implicit Runge-Kutta, DASSL integrator and the Bulirsch-Stoer method; both implicit and explicit.

The results show that the explicit Bulirsch-Stoer method provides the best combination of robustness and speed. However to make the code as adaptable as possible, the existing integrator, the LSODE code and the Bulirsch-Stoer method are to be offered as options to the user. This implementation is currently underway.

Upon completion of the new coding, the eddy-breakup model will be implemented in the NCC. This will be accomplished in the July-August timeframe.

The task of performing a full, 3D reacting simulation of the Sandia D flame was postponed until the end of this year, because of grid issues. The problem was in the resolution at the tip of the jet and pilot tubes. To overcome this, a new grid is being created that treats the tube tips as points, rather than flats. This is expected to have a negligible effect on the flow, as the walls are very thin, but should prevent the convergence problems of the old grid.

**December 16, 2001–December 16, 2002**

***ZCET Program***

For the ZCET program, a 3D simulation of the Sandia Combustor was performed with updated inlet conditions. The results are pending.

***NOx Post-Processing***

For the NOx post-processing, the ILDM based post processor was applied to a swirling dump combustor, and also calibrated with the experimental data. Overall the performance

was disappointing, with significant over-prediction of the NOx levels. Following on from this, a PSR based post processor was developed and also calibrated against the experimental data. This process under predicted the NOx levels, which because of the neglect of convective modeling, was to be expected. Coupling the PSR NOx predictor with a convective model is the next step and is expected to provide good results.

*NPSS GE90 Full Engine Simulation*

For the NPSS program, code modifications for the source-sink terms were included in the main NCC release. In addition, the ability to model effusive cooling flows was added as well as some minor bug fixes. Data from last years GE90 full engine run is being provided to the Visualization Laboratory, who will be developing a full 3D interactive model of the engine.

*Model Development*

For the code development work, a scalar Assumed PDF model (based on the work of S. Girimaji) was implemented in the NCC. Part of this work also involved creating a new data structure to enable the chemistry models to be switched during a simulation, rather than restarting each time. This will enable the development of an NCC convective post-processor and also provide significant speedup in computing time for reacting flow calculations, by starting with simple chemistry models, and switching to more complex as convergence is reached. Various other small fixes and modifications to support other projects were also performed.

**December 16, 2002–December 16, 2003**

*NPSS GE90 Full Engine Simulation*

For this project, the NCC was modified to include a full set up mass source-sink boundary conditions for the purpose of providing models for effusion cooling and also treating exit boundary conditions with a fixed mass flow. The grid for the GE90 combustor was then modified and tested with the new boundary conditions. Working on integrating this into the NPSS cycle code is still ongoing.

*RANS-LES*

The Linear Eddy Model for combustion was evaluated in the 1D test code. Currently the 3D model is being evaluated in the RANS model, and will be put in the LES model soon. Considerable effort is being made to ensure that the transition between RANS and LES is accomplished with consistent time and length scales, to ensure an accurate comparison between the two codes.

### *Model Development*

The implementation of the three-stage Magnussen model written by Marek et al was accomplished. Further validation work is also required on this project. In addition a pre-processor was written that allows the user to switch between different combustion models while the code is being run. This code automatically adds or subtracts species from the restart files and checks all the boundary conditions for consistency.

### *NOx Post Processor*

A stand-alone post processor was tested on the NCC to allow the prediction of NOx values. However the performance was not very good, and so a more sophisticated model was proposed and is being implemented into NCC. This model involves using the NCC solver to update certain species while holding other properties constant. Coding for this is currently being worked on.

### *Publications*

M.G. Turner, A.T. Norris and J.P. Veres, *High-Fidelity Three-Dimensional Simulation of the GE90*, NASA Lewis Research Center, Cleveland OH, NASA Technical Memorandum 212981, 2003

T.-H. Shih, T.D. Smith, C.J. Marek, A. Iannetti, A.T. Norris and N.-S. Liu, *Numerical Study of a Single Hydrogen/Air Gas Turbine Fuel Nozzle*, AIAA 33rd Fluid Dynamics Conference and Exhibit, Reno, Nevada, AIAA-2003-4249, 2003

### Summary

During the lifetime of this grant, work has been performed in the areas of model development, code development, code validation and code application.

For model development, this has included the PDF combustion module, chemical kinetics based on thermodynamics, neural network storage of chemical kinetics, ILDM chemical kinetics and assumed PDF work. Many of these models were then implemented in the code, and in addition many improvements were made to the code, including the addition of new chemistry integrators, property evaluation schemes, new chemistry models and turbulence-chemistry interaction methodology.

Validation of all new models and code improvements were also performed, while application of the code to the ZCET program and also the NPSS GE90 combustor program were also performed.

Several important items remain under development, including the NOx post processing, assumed PDF model development and chemical kinetic development. It is expected that this work will continue under the new grant.